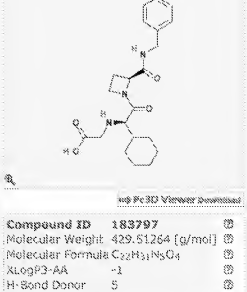
melagatran - Compound Summary (CID 183797)

» Structure & Quick Link Bar

2D 3D



Jmol PC3D Viewer Download

RN refers to (R-(2S))-isomer; ximelagatran is a prodrug that is hydroxylated to melagatran as active thrombin inhibitor

Table of Contents

- BioMedical Annotation
  - Pharmacological Action
  - Pharmacological Classification
  - Chemical Classification
  - Literature Links
  - Literature Mining
- BioAssay Results
- Protein Structures
- Synonyms
- Properties
- Descriptors
- Compound Information
- Substance Information
  - Category
- Exports

Compound ID	**183797**
Molecular Weight	429.51264 [g/mol]
Molecular Formula	$C_{22}H_{31}N_5O_4$
XLogP3-AA	-1
H-Bond Donor	5
H-Bond Acceptor	7

BioMedical Annotation: (Total:1)

melagatran

Pharmacological Action

Anticoagulants · Agents that prevent blood clotting. Naturally occurring agents in the blood are included only when they are used as drugs.

Pharmacological Classification

Chemical Actions and Uses
- Pharmacologic Actions
  - Therapeutic Uses
    - Hematologic Agents
      - **Anticoagulants**

Related Chemical Classification

- Heterocyclic Compounds
  - Heterocyclic Compounds, 1-Ring
    - Azetines
      - Azetidines
- Organic Chemicals
  - Amines
    - Benzylamines
  - Hydrocarbons
    - Hydrocarbons, Cyclic
      - Hydrocarbons, Aromatic
        - Benzene Derivatives
          - Benzyl Compounds
            - Benzylamines

Literature

Literature Keyword Mining Tool

Links

Protein Structure (3)
NLM Toxicology Link

Chemical Structure Search
BioActivity Summary:
This Compound
with Similar Compounds

Related Compounds:
Same, Connectivity: 4 Links

Similar Compounds: 47 Links
Similar Conformers: 7 Links
View Conformers

Substances:
All: 31 Links
Same structure: 16 Links
Mixture: 15 Links

BioAssay Results:

Tested in BioAssays: All: 1 Active: 1
BioActivity Summary: This Compound with Similar Compounds

AID: 1811 **Source:** Shanghai Institute of Organic Chemistry DataTable
Experimentally measured binding affinity data derived from PDB

Protein Structures: (Total: 2)

MMDB ID: 19511 **PDB ID:** 1K22
Human Thrombin-Inhibitor Complex
Taxonomy: Homo sapiens

MMDB ID: 17971 **PDB ID:** 1K1P
Bovine Trypsin-Inhibitor Complex
Taxonomy: Bos taurus

Depositor-Supplied Synonyms: (Total: 23)

Display: Next 10 | All | Sort: Weight

Melagatran
Exanta
Melagatran (INN)
Melagatran AstraZeneca
UNII-2A9QP32MO4
MELAGATRAN (ASTRA-ZENECA)
1k22
CHEBI:102451
MolPort-003-848-481
C22H31N5O4

Properties Computed from Structure:

Molecular Weight	429.51264 [g/mol]
Molecular Formula	$C_{22}H_{31}N_5O_4$
XLogP3-AA	-1
H-Bond Donor	5
H-Bond Acceptor	7
Rotatable Bond Count	9
Tautomer Count	2
Exact Mass	429.237605
MonoIsotopic Mass	429.237605
Topological Polar Surface Area	149
Heavy Atom Count	31
Formal Charge	0
Complexity	671
Isotope Atom Count	0
Defined Atom StereoCenter Count	2
Undefined Atom StereoCenter Count	0
Defined Bond StereoCenter Count	0
Undefined Bond StereoCenter Count	0
Covalently-Bonded Unit Count	1

Descriptors Computed from Structure:

IUPAC Name: 2-[[(1R)-2-[(2S)-2-[(4-carbamimidoylphenyl)methylcarbamoyl]azetidin-1-yl]-1-cyclohexyl-2-oxoethyl]amino]acetic acid
Canonical SMILES:
C1CCC(CC1)C(C(=O)N2CCC2C(=O)NCC3=CC=C(C=C3)C(=N)N)NCC(=O)O
Isomeric SMILES: C1CCC(CC1)[C@H](C(=O)N2CC[C@H]2C(=O)NCC3=CC=C(C=C3)C(=N)N)NCC(=O)O
InChI: InChI=1S/C22H31N5O4/c23-20(29)16-8-6-14(7-9-16)12-26-21(30)17-10-11-27-17)22(31)19(25-13-18(28)29)15-4-2-1-3-5-15/h6-9,15,17,19,25H,1-5,10-13H2,(H3,23,24)(H,26,30)(H,28,29)/t17-,19+/m0/s1
InChIKey: DKWNMCUOEDMMIN-PKOBYXMFSA-N

Compound Information:

CID 183797
Create Date: 2005-06-24

Related Compounds:
Same, Connectivity: 4 Links

Similar Compounds: 47 Links
Similar Conformers: 7 Links View Conformers

Substance Information:

Substances:
All: 31 Links
Same structure: 16 Links
Mixture: 15 Links

Category: [for same structure substances]
Biological Properties: 7 Links
BindingDB (1)
SID 81054817 - External ID: 29388
ChEBI (1)
SID 85308039 - External ID: CHEBI:102451
ChemSpider (1)
SID 33506196 - External ID: 159822
DiscoveryGate (1)
SID 10260002 - External ID: 183797
LeadScope (1)
SID 49973260 - External ID: LS-72219
NextBio (1)
SID 75448641 - External ID: 183797
Shanghai Institute of Organic Chemistry (1)
SID 46392332 - External ID: 1k22

Chemical Reactions: 1 Link
ChemSpider (1)
SID 33506196 - External ID: 159822

Journal Publishers: 3 Links
Prous Science Drugs of the Future (1)
SID 12015035 - External ID: 233311
Thomson Pharma (2)
SID 14807481 - External ID: 00001847
SID 14832162 - External ID: 00043823

Metabolic Pathways: 1 Link
KEGG (1)
SID 51091482 - External ID: D07143

Physical Properties: 1 Link
ChemSpider (1)
SID 33506196 - External ID: 159822

EXHIBIT A

Protein 3D Structures: 3 Links
MMDB (2)
SID 623967 - External ID: 17971.3
SID 623976 - External ID: 19511.8
SMID (1)
SID 7868877 - External ID: MEL

Substance Vendors: 1 Link
MolPort (1)
SID 91614282 - External ID: MolPort-003-848-481

Theoretical Properties: 1 Link
ChemSpider (1)
SID 33506196 - External ID: 159822

Toxicology: 1 Link
ChemIDplus (1)
SID 761147 - External ID: 159776702

ASN.1 XML SDF